Mohsen Kompany-Zareh Associate Prof. of Analytical Chemistry

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BIRTH: Sept 2nd, 1967(Shiraz, Iran), STATUS: Married,

CHILDREN: one son.

Fields interests

Application of

Factor based methods (PCA, PCR, PLS, GRAM, MCR-ALS, PARAFAC, TUCKER), artificial intelligence based techniques (Kohonen map, Radial basis function networks, Genetic algorithms), and signal processing procedures (Wavelet transform)

in

Kinetic and equilibrium studies (Interaction of DNA with small drug molecules), multivariate calibration, pattern recognition and classification (disease diagnosis and metabolic studies), quantitative structure-property/activity relationship QSAR/QSPR (study the class of anti-HIV drugs).

Using the data from

UV-Vis Spectrophotometer, Excitation-Emission Spectrofluorimeter, NearIR spectrometer, Nuclear magnetic resonance, FT-Raman, and simple hand scanner. [Molecular descriptors, generated from different softwares are the applied in QSAR/QSPR].

EDUCATION:

Muti-way Analysis course (by: Rasmus Bro and Frans van den Berg), University of Copenhagen, Denmark [Jan 2008].

Shahid Beheshti University, College of Sciences 19839, Evin, Tehran, Iran.

Degree: PhD in Analytical Chemistry [Jun 1998].

Thesis: Simultaneous spectrophotometric determination of metals in some alloys using Artificial Neural Networks and Factor Analysis techniques.

Shiraz University, College of Sciences 71454, Shiraz, Iran.

Degree: M.S. in Analytical Chemistry [Jun 1993].

Thesis: Extraction-fluorimetric and extraction-spectrophotometric determination of mercury and lead by diaza-18-crown-6 and rose Bengal.

Degree: **<u>B.S.</u>** in Chemistry [Feb 1991]

HOUNORS AND SCHOLARSHIPS:

Outstanding Researcher of State (2004) Top score student in B.S. degree. Second score student in M.S. degree. Scholarship: Iran Ministry of Sciences, Research, and Technology [PhD]

GRADUATED STUDENTS

Yousef Akhlaghi (M.S. in Analytical Chem., Nov 2003) Siavash Mizaei (M.S. in Analytical Chem., Feb 2004) Maryam Khoshkam(M.S. in Analytical Chem., Nov 2006)

MICELANEOUS

Taking part in Design of Webpage of Chemistry Department, 2004.

CONFERENCES, Recent (poster or oral presentation)

- xi- R. Romano, J. S. Vestergaard, M. Kompany-Zareh, W. L. P. Bredie ,Monitoring panel performance within and between sensory experiments by multi-way analysis, First joint meeting of the société francophone de classification and the classification and data analysis group of Italian statistical society, Caserta, Italy, 11-13 June, 2008. (http://orgprints.org/14718/)
- x- European Science Conference on Process Analytical Technology 2 (EuPAT2), Copenhagen, Denmark 2007.
- ix- S. Mirzaei and M. Kompany-Zareh, Resolution of ternary mixtures of pseudoephedrine hydrochloride, dextromethorphan hydrobromide, and sodium benzoate in syrups using wavelength selection by net analyte signals calculated with hybrid linear analysis, The First Seminar of Medicinal & Natural Products Chemistry, Shiraz University of Medical Sciences, Shiraz, Iran, May 2005.
- viii- Y. Akhlaghi and M. Kompany-Zareh, QSAR study of water solubility of saturated alcohols using Artificial Neural Networks, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, Iran, Feb 2004.

- vii- Y. Akhlaghi and M. Kompany-Zareh, t-HPSAM in a nonlinear spectrophotometric system for simultaneous determination of copper and zinc, 14th Iranian Chemistry and Chemical Engineering Congress, Tarbiat Moallem University, Tehran, Iran, Feb **2004**.
- vi- S. Mirzaei, and M. Kompany-Zareh, Genetic algorithm based method for selecting conditions in multivariate determination of povidone-iodine using hand scanner, 12th Iranian Seminar of Analytical Chemistry, Mazandaran University, Babolsar, Iran, Jan **2003**.
- v- S. Farrokhi-kurd, M. Kompany-Zareh, Genetic algorithm applied to condition selection in simultaneous quantification of three food colorants using a hand-scanner, 12th Iranian Seminar of Analytical Chemistry, Mazandaran University, Babolsar, Iran, Jan 2003.
- iv- M.Kompany-Zareh, A. Safavi, and M. Hoseiny, Simultaneous spectrophotometric determination of copper(II) and zinc(II) using partial least squares regression, 12th Iranian Seminar of Analytical Chemistry, Mazandaran University, Babolsar, Iran, Jan 2003.
- iii- M. Kompany-Zareh and H. Tavallali, Generalized artificial neural networks coupled with an orthogonal design to optimization of a system for the kinetic spectrophotometric determination of Hg(II), 11th Iranian Seminar of Analytical Chemistry, Yazd University, Yazd, Iran, Jan 2002.
- ii- M. Kompany-Zareh, M. Mansourian, and F. Ravaee, Colorimetric spot-test quantitative analysis of Fe(III) using a computer controlled hand-scanner, 11th Iranian Seminar of Analytical Chemistry, Yazd University, Yazd, Iran, Jan 2002.
- i- M. Kompany-Zareh, H. Tavallali, and A. Massoumi, Simultaneous Spectrophotometric Determination of Copper(II) and Nickel(II) as Complexes with Sodium Diethyldithiocarbamate in an Anionic Micellar Media Using Partial Least-Squares Regression, 10th Iranian Seminar of Analytical Chemistry, Sharif University, Tehran, Iran, Feb **2001**.

LECTURES:

- 8th Iranian Chemometrics Workshop, Feb, 2009, Zanjan.
- 6th Iranian Chemometrics Workshop, Sep, 2006, Zanjan.
- 5th Iranian Chemometrics Workshop, Sep, 2005, Zanjan.
- 4th Iranian Chemometrics Workshop, Sep, 2004, Zanjan.
- "Direct Exponential Curve resolution algorithm", Department meetings at IASBS, 2004
- 3rd Iranian Chemometrics Workshop, Aug, 2003 (As lecturer)
- "Partial Least Squares", 2nd Iranian Chemometrics Workshop, Sep, 2002
- "3D QSAR using PARAFAC and TUCKER", 1st Iranian Chemometrics Workshop, Sep, 2001

STAYS ABROAD

June 2006-August 2006: Two months stay in Chemometrics Group of Bristol University, England; Process monitoring studies on the data from GlaxoSmithKline (GSK); cooperation with professor Richard Brereton; Supported by Iranian government.

November 2007-May 2008: Six months sabbatical leave in chemometrics group of Quality and Technology section at the Department of Food Science, University of Copenhagen, Denmark; cooperation with professor Rasmus Bro in Multi-way analysis, Bootstrap and Discrete Wavelet studies on Raman and fluorescence data.

EXECUTIVE

- Executive manager of 8th Iranian Chemometrics Workshop, 7-9 Feb, 2009, Zanjan.
- Dean of Central Libray of Yasuj Univ. (2 years

PROFESSIONAL EXPERIENCE

Institute for Advanced Studies in Basic Sciences (IASBS) [Sep 2001 till present]

- 1. Teaching (courses):
 - Advanced analytical chemistry
 - Advanced electrochemistry (I)
 - Advanced electrochemistry (II)
 - Separation II (chromatography)
 - Advanced Analytical Spectroscopy I (Introduction)
 - Advanced Analytical Spectroscopy II (Atomic)
 - Advanced Analytical Spectroscopy III (Molecular)
 - Advanced statistics (for PhD students)
- 2. Research : Application of Chemometrics techniques in
 - QSAR and QSPR
 - Equilibrium and kinetic spectrophotometric studies
 - Multivariate calibration using scanner

Yasuj University [Oct 1998 to Sep 2001]

- 1. Teaching (courses and laboratories):
- Analytical chemistry, organic chemistry, electrochemistry, and instrumental analysis 2. Research in:
 - Application of new chemometrics methods in QSAR
 - Application of Experimental Design in kinetic spectrophotometric determinations
 - Semiquantitative studies, using scanner

Shahid Beheshti University [as PhD candidate]

Teaching assistant for: General chemistry, analytical chemistry and instrumental analysis courses and laboratories

Shiraz University [During M.S.]:

- 1. Teaching assistant for General chemistry and analytical chemistry courses and laboratories
- 2. Research in:
 - Optimization of molecular conformations using MOPAC package
 - Programming with MATLAB and QBASIC, EXCEL for chemical applications

PUBLICATIONS :

------ M.S. ------

- 1. M. Shamsipur, M. Kompany, Extraction-Fluorimetric Determination of trace amounts of mercury by 1,10-Diaza-18-crown-6 and Rose Bengal, *Iran. J. Chem. & Chem. Eng.* 14(**1995**), 2, 59-64.
- 2. M. Shamsipur, M. Kompany, Extraction-Spectrophotometric Determination of trace amounts of lead by 1,10-Diaza-18-crown-6 and Rose Bengal, J. Sci. I.R. Iran 7(1996)1, 13-16.

----- PhD ------

- 3. M. Kompany-Zareh and A. Massoumi, Multicomponent Determination of Cobalt, Copper, and Iron with 1,10-Phenanthroline by Principal Component Regression Modeling of Spectrophotometric Data, *Fresenius' J. Anal. Chem.* 363(**1999**)3, 219-223.
- 4. M. Kompany-Zareh and A. Massoumi, Simultaneous Spectrophotometric Determination of Fe and Ni With Xylenol Orange Using Principal Component Analysis and Artificial Neural Networks in Some Industrial Samples, *Talanta* 48(**1999**)2, 283-92.
- 5. M. Kompany-Zareh, H. Tavallali, and A. Massoumi, Simultaneous Spectrophotometric Determination of Copper(II) and Nickel(II) as Complexes with Sodium Diethyldithiocarbamate in an Anionic Micellar Media Using Partial Least-Squares Regression, *Microchem. J.* 63 (1999) 2, 257-265.

------ Yasuj Univ ------

- 6. M. Kompany-Zareh, Ali Massoumi, and H.Khajehsharifi, Spectrophotometric Multicomponent Analysis of Metals by a Simply Improved Multiple Linear Regression Technique, *American Lab.* (2000) Dec, 20-22.
- 7. M. Kompany-Zareh, M. Latif, A.E. Afshar and A. Massoumi, Simulation of ¹H Nuclear Magnetic Resonance Spectra of Some Organic Compounds Using Artificial Neural Networks, *American Lab. News* (2001) May, 60-61.

------ Institute for Advanced Studies in Basic Sciences ------

- 8. M. Kompany-Zareh, M. Mansourian, and F. Ravaee, A simple method for colorimetric spot-test quantitative analysis of Fe(III) using a computer controlled hand-scanner', *Anal. Chim. Acta*, 471(**2002**) 97-104.
- 9. M. Kompany-Zareh, H. Tavallali, and M. Sajjadi, Application of generalized artificial neural networks coupled with an orthogonal design to optimization of a system for the kinetic spectrophotometric determination of Hg(II), *Anal. Chim. Acta* 469(**2002**) 303-310.
- 10. M. Kompany-Zareh, QSAR study of water solubility of saturated alcohols using Artificial Neural Networks. , *Acta Chim. Slov.*, 50 (2003), 259-273.
- 11. M.Kompany-Zareh, A. Safavi, and M. Hoseiny, Simultaneous spectrophotometric determination of copper(II) and zinc(II) using partial least squares regression, *Chemical Analysis* 49 (2004) 225-234.
- 12. A. Afshar-Ebrahimi, M. Kompany-Zareh, and A. Massoumi, Simultaneous spectrophotometric determination of iron, nickel ,and vanadium using partial least-squares regression, *CHEMIA ANALITYCZNA* 49 (**2004**) 3, 413-420.
- 13. Y. Akhlaghi and M. Kompany-Zareh, Employment of t-HPSAM in a nonlinear spectrophotometric system for simultaneous determination of copper and zinc, *Microchimica Acta*, 148 (**2004**)1-2, 77-85.
- Mohsen Kompany-Zareh, Siavash Mirzaei, Spectrophotometric resolution of ternary mixtures of pseudoephedrine hydrochloride, dextromethorphan hydrobromide, and sodium benzoate in syrups using wavelength selection by net analyte signals calculated with hybrid linear analysis, *Anal. Chim. Acta*, 526 (2004)1, 83-94.
- M. Kompany-Zareh, S. Mirzaei, Genetic algorithm based method for selecting conditions in multivariate determination of povidone-iodine using hand scanner, *Anal. Chim. Acta*, 521(2004) 231-236.

- 16. S. Farrokhi-kurd, M. Kompany-Zareh, Genetic algorithm applied to condition selection in simultaneous quantification of three food colorants using a hand-scanner, *Microchimica Acta*, (2005), 150, 77-86.
- 17. Y. Akhlaghi , M. Kompany-Zareh, Comparing radial basis function and feed-forward neural networks assisted by linear discriminant or principal component analysis for simultaneous spectrophotometric quantification of mercury and copper, *Anal. Chim. Acta* 537 (**2005**) 1-2, 331-338.
- 18. Yousef Akhlaghi, Mohsen Kompany-Zareh, Application of radial basis function networks and successive projections algorithm in a QSAR study of anti-HIV activity for a large group of HEPT derivatives. *J. Chemometr.* 20 (**2006**) 1-12.
- 19. Mohsen Kompany-Zareh and Yousef Akhlaghi, Correlation Weighted Successive Projections Algorithm as a novel method for variable selection in QSAR Studies: Investigation of Anti-HIV Activity of HEPT Derivatives. J. Chemometr. 21 (2007)239-250.
- 20. Mohsen Kompany-Zareh and Mehdi Vasighi, Application of rank annihilation factor analysis in resolution of NIR spectral data from distillation of binary mixture of solvents, *Fuel Processing Technology*, 89 (2008) 203-213.
- 21. Mohsen Kompany-Zareh and Maryam Khoshkam, Application of chemometrics methods with kinetic constraints for estimation of rate constants of second order consecutive reactions. *Anal. Sci.* **2008**, 24, 637-645.
- 22. Mohsen Kompany-Zareh and Yaser Beyad, Target transform fitting in a voltammetric study of metal complexation, *Anal. Chim. Acta* 621 (**2008**) 163-170.
- 23. Mohsen Kompany-Zareh and Mehdi Vasighi, Analysis of solvents mixtures employing rank annihilation factor analysis on near infrared spectral data from sequential addition of analyte, *Fuel Processing Technolog.* 2009, accepted.
- 24. M. Kompany-Zareh, An improved QSAR study of the toxicity of aliphatic carboxylic acids using genetic algorithm. *Med Chem Res* 18 (2009) 143-157.
- 25. Mohsen Kompany-Zareh and Somayyeh Gholami, Parallel vector analysis based soft resolution of spectral data from pH-metric titration using symmetry constraint, *J Chemometr*, 2009 accepted.
- 26. Mohsen Kompany-Zareh and Maryam Khoshkam, QSAR modeling of dihydrofolate reductase inhibitors' activities based on optimization of correlation weights of local graph invariants (CWLGI) using genetic algorithm, *J molecular graphics and modeling* submitted.
- 27. Rosaria Romano and Mohsen Kompany-Zareh, Monitoring panel performance within and between sensory experiments by multi-way analysis, , in preparation.
- 28. Mohammad Arjmand, Mohsen Kompany-Zareh, Mahdi Vasighi, Nastran Parvizzadeh, Zahra Zamani and Fereshteh Nazgooei, 1H NMR based metabolomics for Thalassemia screening and quantification of some hematological parameters using chemometric methods, submitted.

29.

References and copy of published papers available upon request.